Surface Reconstruction of O(2x1)/Cu[110] : A Complete Structural Characterization by Scanned-Energy Photoelectron Diffraction

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INTRODUCTION

The chemisorption of oxygen on Cu (110) is well known to give rise to a reconstruction of the surface Cu atoms. In particular, the oxygen-induced structural change of Cu atoms in the uppermost layers has been studied exhaustively over the last couple of decades, and is now generally believed to result in a missing-row structure.[1] However, the position of oxygen and the interlayer spacing between the topmost surface layers of Cu is not still known with any certainty. Even though many different experimental techniques have been used to investigate this simple, yet intriguing, system, the results of different measurements have often proven to be inconsistent with one another.[2,3,4]

In this study, we have determined the several structural parameters that are under debate for this system with two well-known and complementary surface structure probes: scanned-energy photoelectron diffraction using synchrotron radiation (also called angle-resolved photoemission fine structure or ARPEFS). The ARPEFS measurements have been performed at Beamline 9.3.2 of the Advanced Light Source (ALS) using the Applied Materials Chamber (AMC). In this experiment, an oxygen 1s intensity has been monitored, thus directly probing the local atomic structure around the adsorbed atom. The ARPEFS data was analyzed using a multiple scattering program developed by Chen et al., with structural parameters being optimized via R factors.

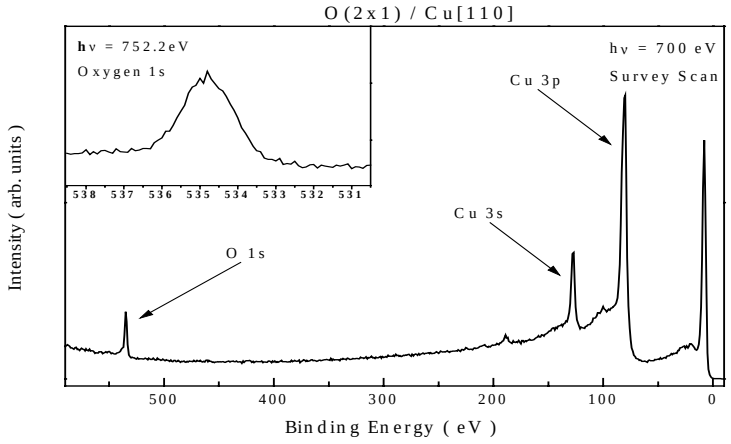

Fig.1. Survey XPS spectrum for O (2X1) / Cu[110] at room temperature with photon energy hν=700 eV. Inset shows the O 1s peak with hν=752.2 eV of which intensities have been scanned with a function of photon energy.

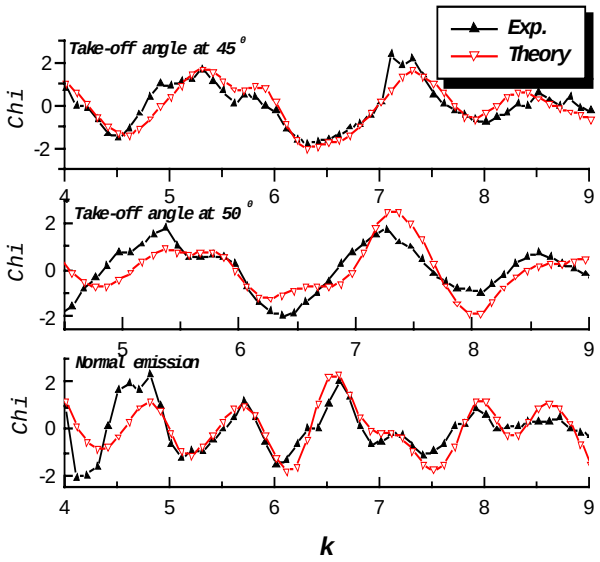

Fig.2. Comparison of experimental data of O 1s ARPEFS in various emissions angles with calculation.

EXPERIMENTAL

The experiment was carried out on bend-magnet beam line 9.3.2 at the Advanced Light Source, using AMC chamber. The Cu[110] sample was cleaned with normal procedures, e.g. Ar bombardment and annealing repeatedly. The clean LEED pattern was observed and the surface cleanness was checked with XPS. [Fig.1] The sample, then, exposed to the oxygen at 10L while the clean (2x1) LEED pattern was being observed at the room temperature. To avoid the CO formation on the surface, the ion gauge filament and ion pump was turned off during the exposure. The LEED pattern was also used as the guiding reference of Cu orientation relative to the polarization of incoming light from the beam line. The pressure of the chamber was kept under the $2x10^{-10}$ torr during the taking data set. The O 1s intensity of various take-off angles was measured while the photon energy was varied, i.e. varying the kinetic energies of O 1s. All spectra were individually fitted with proper background subtraction. [Fig.2]

CONCLUSION

We found in the analysis that photoelectrons with very low take-off angles with respect to the surface (≤ 12 degree) are subject to highly preferential scattering events along the emitter-detector direction, and that correctly including enough scatters along such directions is crucial for accurately simulating the experimental data with multiple-scattering theory. From this analysis, it is found that the adsorbed oxygen atoms are positioned slightly below the topmost Cu layer ($d_0 = 0.075$Å), and this placement leads to an increase of the interlayer spacing between the two top layers of copper ($d_{12} = 1.565$Å, *compared to 1.287 Å* in bulk Cu). Our XPD results in the low takeoff angle region have also been analyzed and their structural implications are compared with those derived via the ARPEFS data.

ACKNOWLEDGMENT

This work was supported by the Director, Office of Science, Office of Basic Energy Sciences, Materials Sciences Division, of the U.S. Department of Energy and the Korea National Science Foundation.

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